

Evaluation of Centroidal Voronoi Tessellation as a Statistical Sampling Method*

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Note to SAMO '04 Selection Committee: the following is a draft paper still under development which is as yet incomplete. If this submission is accepted for the conference this draft will be expanded into a full paper reflecting the scope of the title above and abstract below.

Abstract

A recently developed Centroidal Voronoi Tessellation (CVT) unstructured sampling method is investigated here to assess its suitability for use in statistical sampling. CVT efficiently generates a highly uniform distribution of sample points over arbitrarily shaped M-Dimensional parameter spaces. It has recently been shown on several 2-D test problems to provide desirable point distributions for function integration, statistical estimation, and for generating locally conforming response surfaces. In this paper, its performance as a statistical sampling method is further compared to that of Latin-Hypercube Sampling (LHS) and Simple Random Sampling (SRS) Monte Carlo methods, and Halton and Hammersley quasi-Monte-Carlo sequence methods. Sampling efficiencies are compared for resolving various statistics of response in a 2-D test problem. It is found that on balance CVT performs best of all these sampling methods on our test problems.

1. Background

For reasons that will become clear later, it is often beneficial in statistical sampling and function integration to sample "uniformly" over the applicable parameter space.

Such uniformity, while conceptually simple and intuitive on a qualitative level, is on a quantitative level somewhat complicated to describe and quantify mathematically. Quantitative aspects of uniformity involve: 1) the equality with which points are spaced relative to one another in the parameter space (are they all nominally the same distance from one another?); 2) uniformity of point density over the entire domain of the parameter space (i.e., uniform "coverage" of the whole domain by the set of points, and not just good uniformity within certain regions of the space); and 3) isotropy in the point placement pattern. Each of these aspects of uniformity can be quantified by several mathematical measures. We will not discuss these measures further here, but we mention them to say that quantitative measures do exist for the intuitive notion of uniformity. We find that in 2-D the visual-intuitive sense of uniformity obtained by viewing a distribution of samples in a square (2-D hypercube) correlates very strongly with the quantitative quality measures mentioned above. Thus, in 2-D the eye is an excellent integrator of the different aspects of uniformity listed above, and a very accurate discriminator of uniformity or lack thereof –or at least in judging whether one particular layout of sample points is more uniform than another.

Much effort has been applied in the literature to the problem of achieving uniform placement of N samples over M-dimensional hypercubes, where M and N are both arbitrary. It is well recognized that Simple-Random sampling (SRS) Monte Carlo does not do a particularly good job of uniformly spreading out the sample points. The popular Latin Hypercube Sampling (LHS) method generally does a much better job of uniformly spreading out the points. This is due to the greater sampling regularity over each individual parameter dimension before the individually generated parameter values are randomly combined

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into parameter sets which define the coordinates of the sampling points ([5]).

Recent efforts to modify LHS to get an even more uniform distribution of points over the parameter space have included Distributed Hypercube Sampling (DHS, [12]) and Improved Distributed Hypercube Sampling (IHS, [2]). The fundamentals and history of these are reviewed in [18]. Though the quantitative measure of uniformity used for comparisons in [2] and [12] was somewhat flawed, it does appear that DHS gives better sampling uniformity than LHS, and that IHS gives better sampling uniformity than DHS but is increasingly more computationally expensive as the dimensionality of the parameter space increases. We have recently become aware of another LHS variant, “Optimal Symmetric LHS” (OSLHS, [21]) which also seems to improve the spatial uniformity of LHS samples. Its computational cost and performance relative to DHS and IHS are not yet known, however.

A number of other potential approaches for achieving uniform point placement that are not evolved from an LHS basis are reviewed (and some new ones are presented) in [7]. There, some quantitative metrics related to visual/sensory perception of point uniformity in 2-D are reviewed and some new ones presented. Many of these non-LHS-based approaches appear to work very well in 2-D, but it is said that some of the methods may not be applicable or may not perform well in more than two dimensions, and some clearly will not scale up to high dimensions affordably. Others seem more promising for high dimensions, but have not yet been investigated enough.

The so-called “Quasi- Monte Carlo” (QMC) quasi- or sub- random low-discrepancy sequence methods (see *e.g.* [14]) can often achieve reasonably uniform sample placement in hypercubes. The strength of these sequence methods (Halton, Hammersley, Sobol, etc.), is that they can produce fairly uniform point distributions even though samples are added one at a time to the parameter space. The one-at-a-time incremental sampling of QMC (and SRS) enables these methods to have better efficiency prospects than CVT and LHS-type methods in the area of error estimation and control. Not only this, the results achieved are often quite good. For resolving the mean and standard deviation of response measures, Hammersley sequences were found in [11] to converge to within 1% of exact results 3 to 100 times faster than LHS over a large range of test problems. For resolving response probabilities, Hammersley and modified-Halton were found in [15] to perform roughly the same as LHS on balance over several test problems.

However, when the hyperspace dimension becomes moderate to large and/or the sampling density becomes high, some (perhaps all?) sequences suffer from spurious

correlation of the samples. This is shown for standard Halton sequences in 16-D (ref. [12]) and 40-D (ref. [15]). Sometimes a modification can be found to suppress or delay the onset of spurious correlation, as a fix from the literature implemented in [15] shows for Halton sequences.

Recently, a long-recognized approach for achieving uniformity of point placement in M-dimensional volumes, called “Centroidal Voronoi Tessellation” (CVT), has been made computationally efficient ([10]) for implementing the principles of Centroidal Voronoi diagrams ([6],[13]). These diagrams subdivide arbitrarily shaped domains in arbitrary-dimensional space into arbitrary numbers of nearly uniform subvolumes, or Voronoi cells/regions. Given a set of N points $\{z_i\}$ ($i=1,\dots,N$) in an M-dimensional hypercube, the Voronoi region or Voronoi cell V_j ($j=1,\dots,N$) corresponding to z_j is defined to be all points in the hypercube that are closer to z_j than to any of the other z_i 's. The set $\{V_i\}$ ($i=1,\dots,N$) is called a Voronoi tessellation or Voronoi diagram of the hypercube, the set $\{z_i\}$ ($i=1,\dots,N$) being the generating points or generators. A *centroidal* Voronoi tessellation (CVT) is a special Voronoi tessellation with the property that each generating point z_i is itself the mass centroid of the corresponding Voronoi region V_i .

Although CVTs are deterministic, they can be converged to with probabilistic sampling methods. In [10], new probabilistic CVT construction algorithms were introduced, implemented, and tested. These methods are generally much more efficient than previous deterministic and probabilistic methods for constructing CVTs.

The CVT concept and the algorithms in [10] for their construction can be generalized in many ways (see [6] for details). For example, instead of a hypercube, general regions in M-dimensional space can be treated. This feature has been exploited with great success (see [6]) for discretizing arbitrary 2-D and 3-D domain volumes for computational mechanics analysis with meshless analogues of finite element methods (*e.g.*, [1]). Furthermore, points can be distributed non-uniformly according to a prescribed density function over the space. For instance, reference [18] shows several CVT point sets spaced according to a bi-Normal joint probability density function. Thus, CVT can be used for Monte-Carlo-like sampling in problems containing multiple random variables. In this regard, we surmise that correlation structure for correlated random variables can be introduced into CVT sampling with the rank correlation procedure [8] employed in [9] for SRS and LHS, and in [11] for Hammersley QMC.

Figure 1 compares three LHS and three corresponding CVT pointsets for 100 samples in a 2D unit hypercube. The three LHS pointsets were generated with [9] for different initial seeds (Seed1 = 123456789, Seed2 = 192837465, Seed3 = 987654321) and a Uniform joint

probability density function over a unit-hypercube parameter space. The three corresponding CVT pointsets were generated ([3]) by using the LHS sets as initial conditions (point locations) to begin the CVT iterations. In all cases the CVT set is much more uniform (visually and quantitatively) than its associated LHS set. All three CVT sets are relatively similar visually and quantitatively, even though starting from three very different initial conditions given by the LHS sets.

The LHS sets exhibit significant clustering and non-uniformity of the points. The LHS sets do not appear to be significantly more uniform than three analogous SRS sets shown in [18], and which will be used here in later comparisons, but quantitatively they are significantly more uniform ([4]). CVT sets from the three different SRS initial sets are shown in [18]. The different LHS and SRS initial conditions do not have much of an impact on final CVT uniformity, so CVT appears to be robust in this regard.

Figures 2 and 3 show Halton and Hammersley pointsets and the corresponding CVT sets started from them. The Halton pointset is noticeably and quantitatively more uniform than any of the LHS sets; the Hammersley set is even more uniform than the Halton set; and the CVT sets are even more uniform than the Hammersley set.

Hence, CVT places samples much more uniformly in the 2D hypercube than SRS and LHS, and even more uniformly than the low-discrepancy Halton and Hammersley QMC sequences. This is true regardless of the initial conditions (sample sets) that CVT starts from ([4]). In initial investigations [4] for 2-D, 7-D, and 20-D test cases, CVT has provided greater sampling uniformity than Halton, Hammersley, Sobol, SRS, LHS, DHS, and IHS according to a meaningful subset of nonflawed quantitative quality measures. Additionally, no degradation of sampling uniformity has been detected in higher dimensions (*i.e.*, for the 20-D case).

It is therefore natural to ask whether CVT can be applied for: A) statistical sampling over arbitrary-dimensional spaces of input random variables to calculate various statistics of output response behavior; B) function integration over arbitrarily shaped domains; and C) whether it can serve as a method for generating favorable point distributions for improved response-surface accuracy.

A preliminary positive indication regarding item C) for response surface generation is presented in [18]. There, CVT was shown on several 2-D test problems to provide superior point distributions for generating locally-conforming Moving Least Squares response surfaces. Point distributions by CVT, SRS, LHS, and a structured sampling method with deterministically uniform point placement ([17]) were tried in the study.

Items A) and B) were initially evaluated in [19] for a 2-D function sampled from a uniform joint density over a 2-D hypercube. The mean and standard deviation of the resulting distribution of function outputs were compared for CVT, SRS, LHS, Halton and Hammersley sampling. CVT yielded the best overall accuracy and precision for the calculated statistics. Under uniform sampling, the connection between function integration and calculation of mean output response was developed, and through this connection it was concluded that CVT should naturally be better than the other sampling methods for function integration.

Certainly, for function integration and point placement for response-surface generation, CVT already appears very promising relative to other structured and unstructured sampling methods. Especially for irregular (non-hypercube) interpolation and integration domains, the regularity of CVT sampling over the domain is a large part of the reason why CVT is already recognized to hold great promise for the application of 2-D and 3-D meshless finite-element methods.

In this paper we concentrate on evaluating CVT as a statistical sampling method. We take a further step by comparing it against SRS, LHS, Halton, and Hammersley for calculating several function response probabilities under uniform sampling, and then for calculating other response probabilities arising from a joint-Normal probability density.

2. Evaluation of CVT as a Statistical Sampling Method

2.1. 2-D Model Problem and Statistical Measures of Response for Performance Evaluation of Sampling Methods

Figure 4 shows an analytic multimodal function describing system response r as a function of two system inputs p_1 and p_2 :

$$r(p_1, p_2) = \left[0.8\kappa + 0.35 \sin\left(2.4\pi \frac{\kappa}{\sqrt{2}}\right) \right] [1.5 \sin(1.3\theta)] \quad \text{EQ 1}$$

on the domain $0 \leq p_1 \leq 1$ and $0 \leq p_2 \leq 1$,

where $\kappa = \sqrt{(p_1)^2 + (p_2)^2}$, $\theta = \text{atan}\left(\frac{p_2}{p_1}\right)$.

A statistical problem arises if p_1 and p_2 are random variables. In that case, any particular realization p_{1i} and p_{2i} of the stochastic variables yields a deterministic response r_i as given by the above functional relationship. An ensemble of responses accompanies the different realizations of p_1 and p_2 as they vary stochastically or randomly

according to their individual propensities, or joint propensities if the two variables are correlated. In probability theory a joint probability density function defined over the input parameter space, JPDF(p_1, p_2), is used to model the relative likelihood of achieving an input combination p_1, p_2 corresponding to the point (p_1, p_2) in the p_1 - p_2 coordinate plane. The JPDF function is defined for every point in the p_1 - p_2 parameter plane and integrates over the plane into a value of unity.

The JPDF likelihood function for attaining various input combinations maps through the response function $r(p_1, p_2)$ into a corresponding likelihood function for response values. Operationally, the resulting response probability density function, PDF(r), can be approached closer and closer via Monte Carlo sampling as more and more parameter sets or realizations $(p_1, p_2)_i$ are randomly generated from the governing input JPDF and are propagated through the response function $r(p_1, p_2)$ into response realizations r_i . The response realizations are distributed in the response space (*i.e.*, along the response coordinate axis r) with a density that, as more and more samples are added, trends toward the exact PDF of response.

Very often, only certain statistical measures of the PDF of response are desired or can be reasonably estimated. Response mean, μ_r , and standard deviation, σ_r , can be estimated directly from the mean $\hat{\mu}_r$ and standard deviation $\hat{\sigma}_r$ of the population or set $\{r_i\}$ of realizations. We have the following definitions:

$$\hat{\mu}_r = \frac{1}{N} \sum_{i=1}^N r_i \quad \text{EQ 2}$$

$$\hat{\sigma}_r = \left[\frac{1}{N-1} \sum_{i=1}^N (r_i - \hat{\mu}_r)^2 \right]^{\frac{1}{2}} \quad \text{EQ 3}$$

where N is the number of realizations or “samples” of response.

Also often of interest is the probability of response exceeding (or not exceeding) some particular threshold value r_T . Exceedence probability is very simply estimated as the ratio of the number of calculated response values at or above the given threshold value, to the total number of samples, N . As the number of response realizations increases, the estimate (quotient) trends toward greater accuracy, *i.e.*, toward the actual exceedence probability. This is of course also true for the estimates $\hat{\mu}_r$ and $\hat{\sigma}_r$ of response mean and standard deviation.

2.2. Comparison of Response Statistics from Various Sampling Methods

Here we compare estimates of response exceedence probabilities as obtained from various sampling methods we have previously introduced: CVT, SRS, LHS, and Halton and Hammersley sequences.

We start with *e.g.* the 100-sample pointsets in Figure 1, which correspond to a uniform JPDF over the input parameter space of our model response function (Figure 4). We map these sets of samples through our response function EQ 1 to obtain corresponding response sets, and then calculate the aforementioned statistics of these populations.

We then compare the calculated statistics of each set to each other and to “reference values” obtained from using three million SRS samples at parameter sets generated by the sampling code [9]. The reference values are actually averages of three results, each obtained from one million samples generated from random initial seeds “X”, “Y”, and “Z” (different from seeds 1, 2, and 3 used to generate the 100-sample LHS sets in Figure 1).

Three “replicate” sets of one million samples each were used in preference to one set of three million samples so that empirical confidence intervals (CI) on the calculated averages could be compared against their classical CI to reaffirm or caveat them. (Recent research ([16], [20]) has shown that for SRS, empirical CI appear to be somewhat more accurate than classical CI.) Empirical CI are formed by assuming the calculated statistic (response mean, standard deviation, or exceedence probability) is a random realization from a Normal or nearly Normal distribution about the exact result. Hence a T-distribution with 3 - 1 = 2 degrees of freedom can be used to get confidence intervals about the small-sample average of the three replicates. Thus, for 95% empirical CI the following formula is used:

$$95\% \text{ confidence half-interval} = 4.303 \frac{\hat{\sigma}_{est}}{\sqrt{3}} \quad \text{EQ 4}$$

where $\hat{\sigma}_{est}$ is the sample standard deviation (*cf.* EQ 3) of the three estimates.

2.2.3. Response Exceedence Probability for $r_T=0.2$. The reference value for exceedence probability (EP) corresponding to a response threshold level of $r_T=0.2$ is $\hat{P}_{ref}=0.870984$. This value is the average of the three EPs calculated from the three 10^6 SRS sets. The standard deviation of these three estimates is $\hat{\sigma}_{est}=0.000257$. Empirical 95% half-CI by EQ 4 are 0.000639. When the reference EP is calculated based on the entire population of $N=3 \times 10^6$ samples, the value doesn’t change from the averaged value based on three separate 10^6 -sample sets, but classical CI can be computed. The classical 95% half-CI from standard statistical formulas is somewhat smaller,

at 0.000379. Using the larger (empirical) 95% half-CI we can then say that at least to 95% certainty the true probability $P_{0.2}$ of response exceeding the threshold value $r_T=0.2$ lies within the range $\hat{P}_{ref} \pm 0.000639 = (0.871623, 0.870345)$.

Since the test sets were limited to 100 sample points, derived probabilities can only be resolved in increments of 0.01. Thus, for the $r_T=0.2$ case, a derived result cannot be more accurate than 0.87 or 0.88 –both of which are equally valid estimates of the true probability, 0.870984 ± 0.000639 , which lies between the attainable values 0.87 and 0.88. In other words, any error in an estimate of 0.87 or 0.88 is due to resolution error from the limited number of samples, and not to a fault or inferiority of the sampling method's point placement scheme or resulting pattern. Hence, in judging the performance of our sampling methods, in Tables 5 and 6 we take results of 0.87 and 0.88 as exact results, and quantify errors therefrom. Accordingly, a sample-set result of *e.g.* 0.89 would entail an error of +0.01 here, and a result of *e.g.* 0.85 would entail an error of -0.02.

From Table 5 we can conclude to well over 95% certainty that the SRS and LHS errors are for all three trials significantly greater than the CVT errors. This is true of individual errors, and for average error magnitude as well (which for CVT is an order of magnitude less than that of SRS and LHS –LHS actually being significantly worse than SRS in this set of trials). The algebraic average of the signed errors shows that the average bias in the LHS and SRS results is similar, and about 50% smaller for CVT. The standard deviation of the estimates is an order of magnitude less for the CVT results than for the LHS and SRS, with SRS significantly better than LHS according to this metric. Thus, in these calculations of exceedence probability, CVT shows an order of magnitude improvement over SRS and LHS in both the error magnitude and standard deviation of the estimates.

Table 6 shows that the Halton error is significantly larger than the Hammersley error. CVT reduces the -0.02 Halton error to zero within our ability to distinguish error here, but does not improve the -0.01 error of the Hammersley result.

2.2.3. Response Exceedence Probability for $r_T=0.5$. The reference value for exceedence probability corresponding to a response threshold level of $r_T=0.5$ is $\hat{P}_{ref}=0.555050$. This value is the average of the three EPs calculated from the three 10^6 SRS sets. The standard deviation of these three estimates is $\hat{\sigma}_{est}=0.000209$. Empirical 95% half-CI by EQ 4 are 0.000519. The reference EP when calculated based on the entire population of $N=3 \times 10^6$ samples yields classical 95% half-CI of 0.000562, very close to the empirical value. Using the larger (classical) 95% half-CI

we can then say to at least 95% certainty that the true probability $P_{0.5}$ of response exceeding the threshold value $r_T=0.5$ lies within the range $\hat{P}_{ref} \pm 0.000562 = (0.555612, 0.554488)$.

Since the test sets were limited to 100 sample points, for the $r_T=0.5$ case a derived result cannot be more accurate than 0.55 or 0.56 –both of which are equally valid estimates of the true probability, 0.555050 ± 0.000562 , which lies between the attainable values 0.55 and 0.56. Hence, in judging the performance of our sampling methods, in Tables 7 and 8 we take results of 0.55 and 0.56 as exact results, and quantify errors therefrom. Accordingly, a sample-set result of *e.g.* 0.57 would entail an error of +0.01 here, and a result of *e.g.* 0.53 would entail an error of -0.02.

From Table 7 we see that the average bias of the SRS samples is an order of magnitude larger for SRS than for LHS and CVT. In the case, LHS bias is smaller than CVT bias by about 50%, but both are small. The standard deviation of the estimates is the same order of magnitude for SRS, LHS, and CVT, with CVT having the smallest standard deviation, then LHS, then SRS. Average error magnitude is also least for CVT, then for LHS, then for SRS.

Table 9 shows that for this problem the Halton error of 0.02 is actually better than the Hammersley error of -0.03. CVT reduces both these errors to zero within our ability to distinguish error here.

3. Closing

Though we have found in very limited testing that CVT typically performs best for calculating means and variances (in [19]) and the various exceedence probabilities above under a uniform JPDE, we have not yet assessed its statistical performance under the much more common situation of non-uniform input random variables. This will be the next important test for CVT, which we plan to assess with the remainder of this paper.

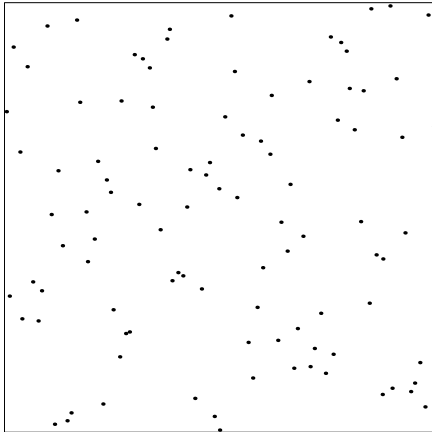
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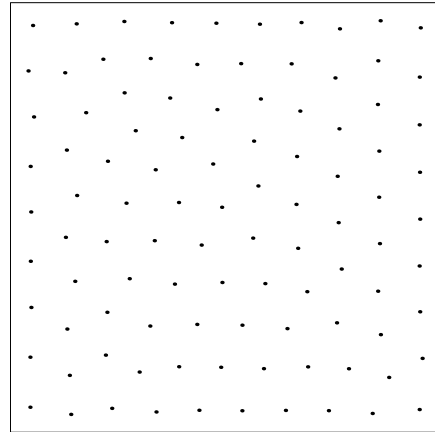
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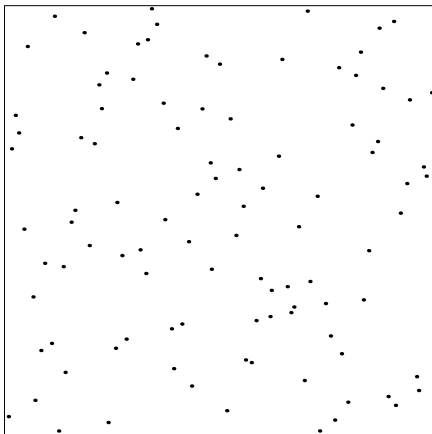
LHS1 pointset (from seed 1)



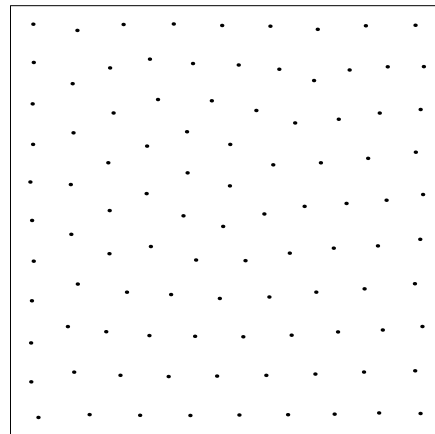
CVT-LHS1 pointset (from LHS1)



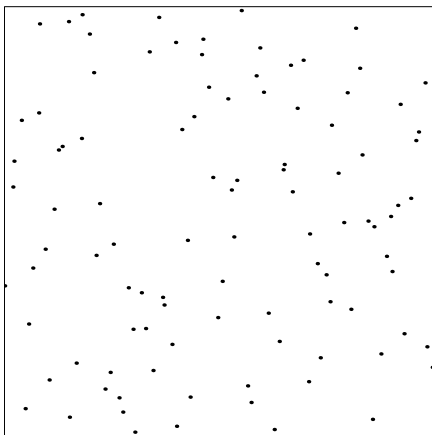
LHS2 pointset (from seed 2)



CVT-LHS2 pointset (from LHS2)



LHS3 pointset (from seed 3)



CVT-LHS3 pointset (from LHS3)

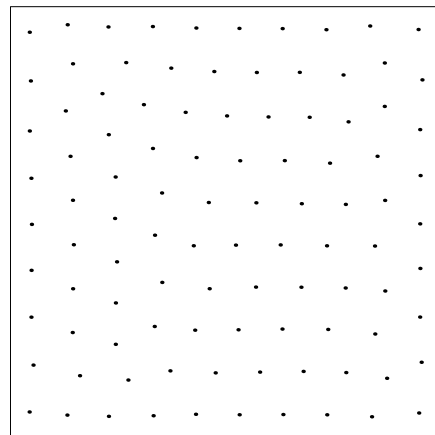


Figure 1. 100-point sample sets on a 2-D unit hypercube for: A) Left Column– uniform JPDP LHS Monte Carlo with three different initial seeds; and B) Right Column– corresponding uniform JPDP CVT sets starting from LHS sets as initial conditions.

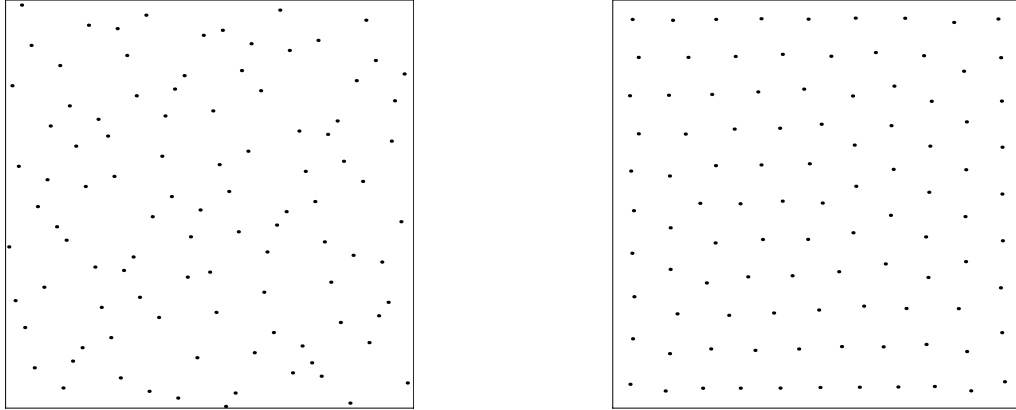


Figure 2. 100-point sample sets on 2-D unit hypercube for:
A) Left plot– Halton QMC sequence;
B) Right plot– corresponding CVT set starting from the Halton set as initial conditions.

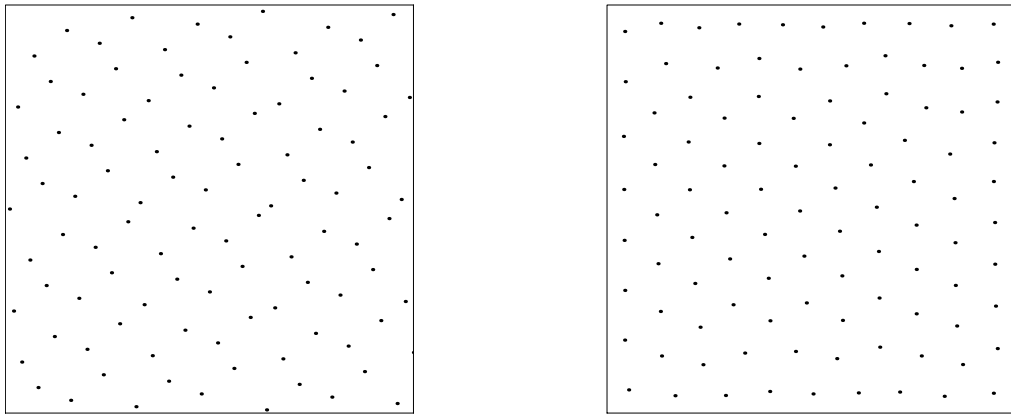


Figure 3. 100-point sample sets on 2-D unit hypercube for:
A) Left plot– Hammersley QMC sequence;
B) Right plot– corresponding CVT set starting from the Hammersley set as initial conditions.

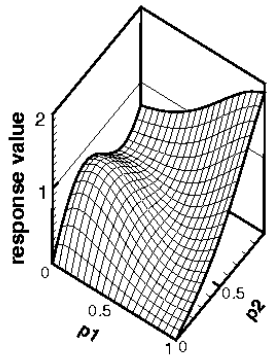


Figure 4. 2-D model function for system response as a function of input parameters p_1 and p_2 .

Table 1. Calculated response exceedence probabilities, threshold=0.2 (100 samples, Uniform 2D JPDF)

		<u>SRS</u>		<u>LHS</u>		<u>CVT</u>	
		$\hat{P}_{0.2}$	$\hat{P}_{0.2}$ error	$\hat{P}_{0.2}$	$\hat{P}_{0.2}$ error	$\hat{P}_{0.2}$	$\hat{P}_{0.2}$ error
REALIZATION	1	0.85	-0.02	0.84	-0.03	0.86	-0.01
	2	0.86	-0.01	0.86	-0.01	0.87	0.0
	3	0.89	+0.01	0.90	+0.02	0.87	0.0
average		0.867	-0.0067	0.867	-0.0067	0.867	-0.0033
std. dev.		0.021	0.0153	0.031	0.0252	0.006	0.0058
avg. error mag.			0.0133		0.02		0.0033

Table 2. Calculated response exceedence probabilities, threshold=0.2 (100 samples, Uniform 2D JPDF)

<u>Halton</u>		<u>Hammersley</u>		<u>CVT</u>	
$\hat{P}_{0.2}$	$\hat{P}_{0.2}$ error	$\hat{P}_{0.2}$	$\hat{P}_{0.2}$ error	$\hat{P}_{0.2}$	$\hat{P}_{0.2}$ error
0.85	-0.02			0.87	0.0
		0.86	-0.01	0.86	-0.01

Table 3. Calculated response exceedence probabilities, threshold=0.5 (100 samples, Uniform 2D JPDF)

		<u>SRS</u>		<u>LHS</u>		<u>CVT</u>	
		$\hat{P}_{0.5}$	$\hat{P}_{0.5}$ error	$\hat{P}_{0.5}$	$\hat{P}_{0.5}$ error	$\hat{P}_{0.5}$	$\hat{P}_{0.5}$ error
REALIZATION	1	0.56	0.	0.53	-0.02	0.55	0.
	2	0.57	+0.01	0.55	0.	0.58	0.02
	3	0.62	+0.06	0.57	+0.01	0.56	0.
average		0.5833	+0.023	0.550	-0.003	0.563	+0.007
std. dev.		0.0321	0.032	0.020	0.015	0.015	0.012
avg. error mag.			0.023		0.01		0.007

Table 4. Calculated response exceedence probabilities, threshold=0.5 (100 samples, Uniform 2D JPDF)

<u>Halton</u>		<u>Hammersley</u>		<u>CVT</u>	
$\hat{P}_{0.5}$	$\hat{P}_{0.5}$ error	$\hat{P}_{0.5}$	$\hat{P}_{0.5}$ error	$\hat{P}_{0.5}$	$\hat{P}_{0.5}$ error
0.58	+0.02			0.56	0.
		0.52	-0.03	0.56	0.